Benzene, 1,2-dichloro-4-isocyanato-

Other names:	3,4-Dichlorfenylisokyanat
	3,4-Dichlorophenyl isocyanate
	3,4-Dichlorphenyl isocyanate
	Isocyanic acid, 3,4-dichlorophenyl ester
Inchi:	InChI=1S/C7H3Cl2NO/c8-6-2-1-5(10-4-11)3-7(6)9/h1-3H
InchiKey:	MFUVCHZWGSJKEQ-UHFFFAOYSA-N
Formula:	C7H3Cl2NO
SMILES:	O=C=Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	188.01
CAS:	102-36-3

Physical Properties

Property code	Value	Unit	Source
chs	-3105.00 ± 4.20	kJ/mol	NIST Webbook
hf	-11.11	kJ/mol	Joback Method
hfs	-119.00 ± 4.20	kJ/mol	NIST Webbook
hvap	53.08	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	2.961		Crippen Method
mcvol	117.460	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	537.73	K	Joback Method
tc	775.74	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	47.40	kJ/mol	423.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30481e+01
Coeff. B	-4.00166e+03
Coeff. C	-5.44450e+01
Temperature range (K), min.	368.04
Temperature range (K), max.	571.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.79002e+02
Coeff. B	-2.85987e+04
Coeff. C	-8.69236e+01
Coeff. D	9.19808e-05
Temperature range (K), min.	316.15
Temperature range (K), max.	526.95

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1803

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1803.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102363&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs: Standard solid enthalpy of combustion

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature